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Title:

PDF-BASED MODELING OF GRAIN-SCALE PROCESSES IN COMPOSIT HIGH EXPLOSIVES

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PDF-based modeling of grain-scale processes in composite high explosives

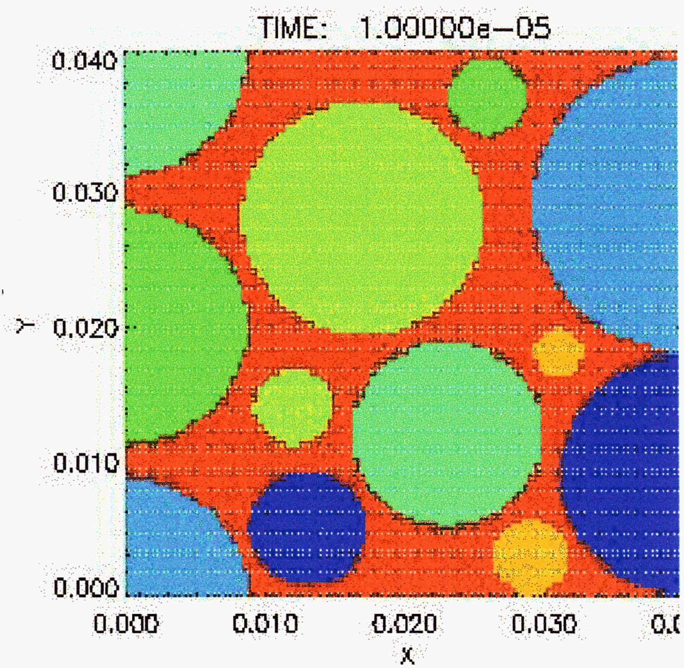
Duan Z. Zhang and Francis Harlow
T-3, LANL

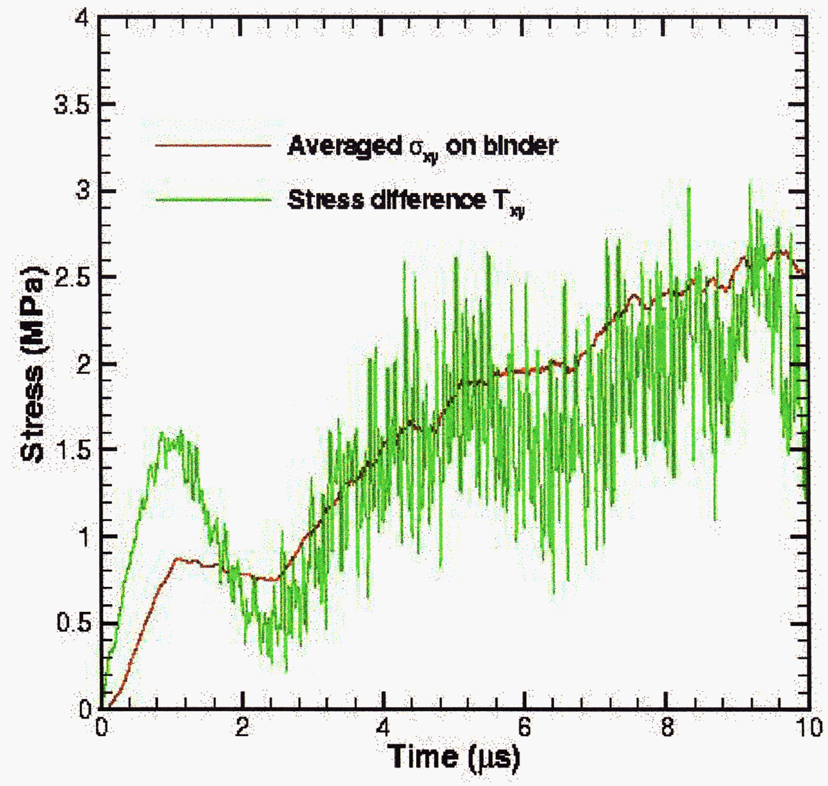
In this talk, we shall review the research activities on high explosive materials during last year. A statistical method is introduced to model the material. Numerical simulations are performed in the microscopic level. Based on the molecular scale interactions, a new constitutive model is obtained and compared with experimental data. We also point out the further research needs.

Micromechanical Processes

- Used statistical micromechanical tools to account for crystal-binder interactions.
- Compared our model prediction with experiment.
- Postulated a phenomenological binder stiffening model and a damage model.
- Identified the need for a better binder model.
- Studied polymer models for high strain rate.

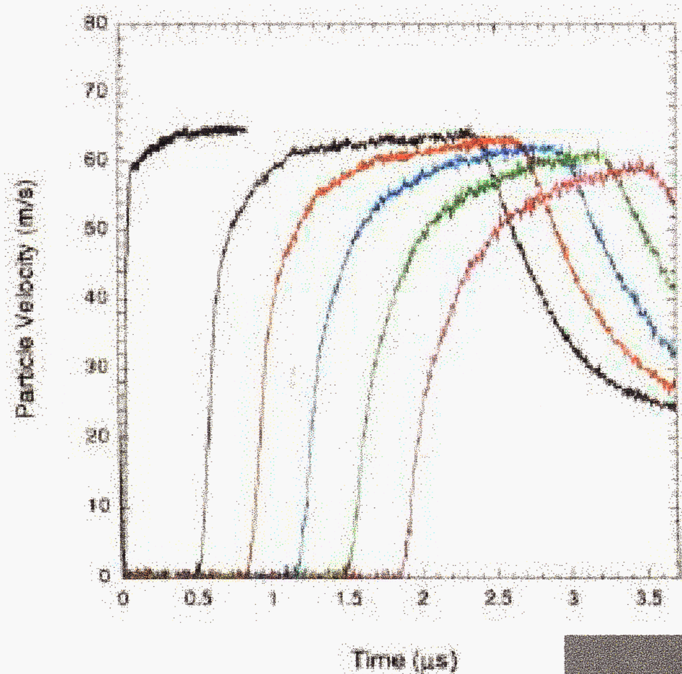
Particle Binder Interactions

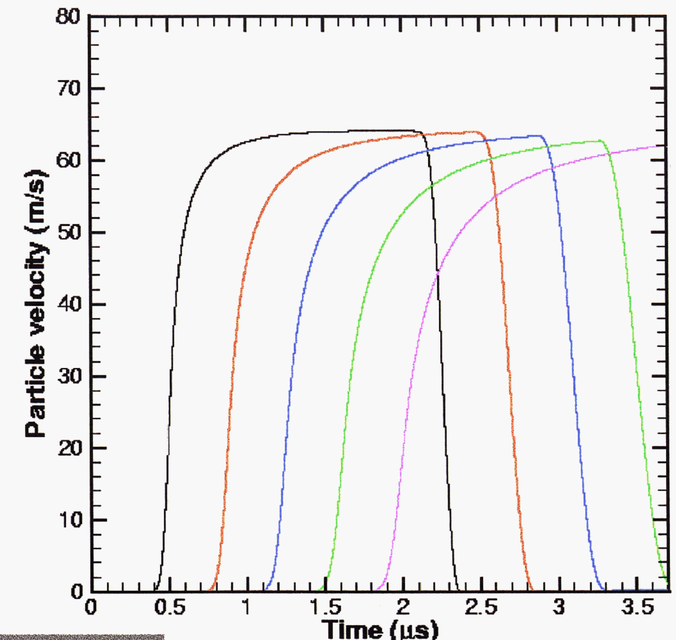


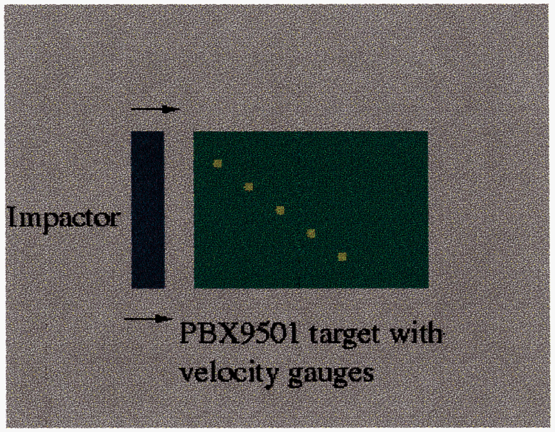


Comparison With Experiment

Particle velocity: 66.1 m/s

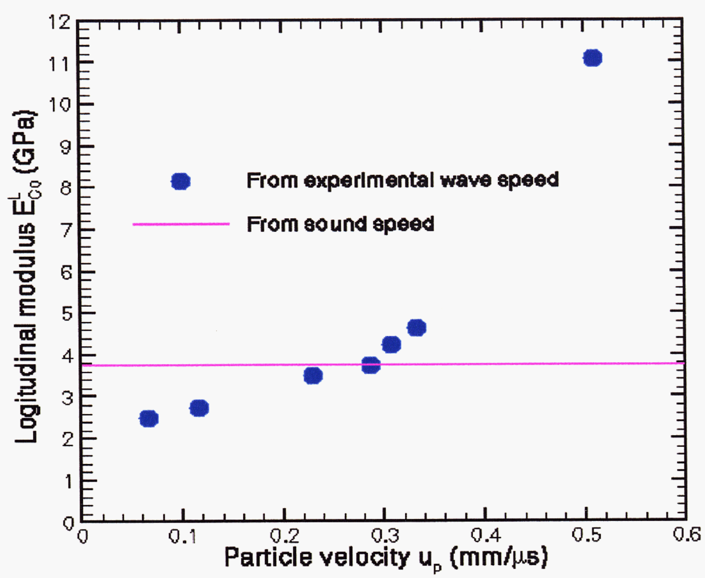






Phenomenological Models for Binder

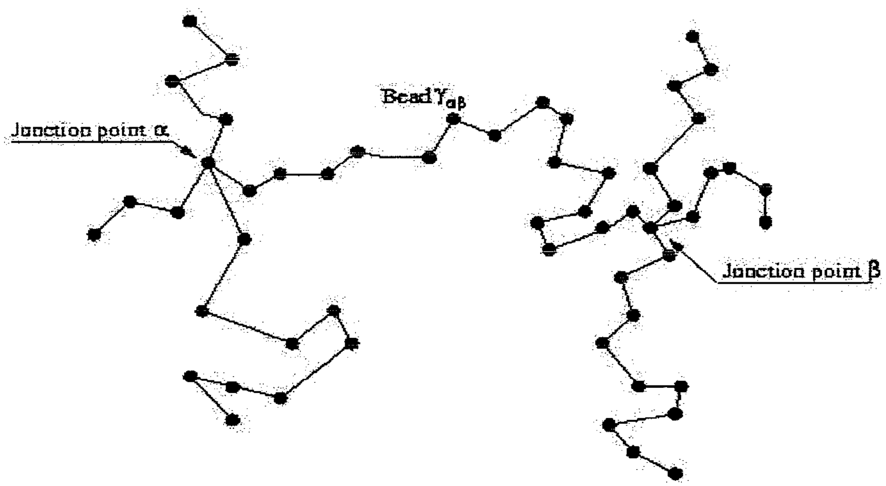
- Stiffening



- Damage and stiffening

$$E_b = [1 - \alpha(\dot{\varepsilon}) \, | \varepsilon |^n] E_0(\dot{\varepsilon})$$

Network Theory for Polymeric Binder Under High Strain Rate

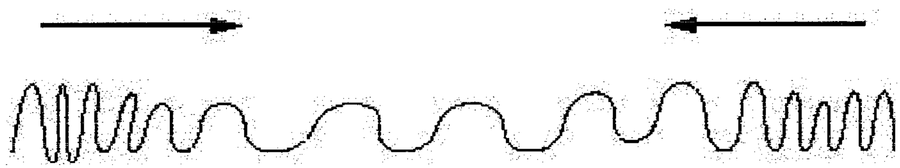


- Derived averaged equations and closure relations for the material based on equation of motion for each individual bead and junction.

- Considers nonequilibrium deformation of polymer chains.

- Chain relaxation time >> (chain length)/(wave speed).

Diffusion waves move toward center.

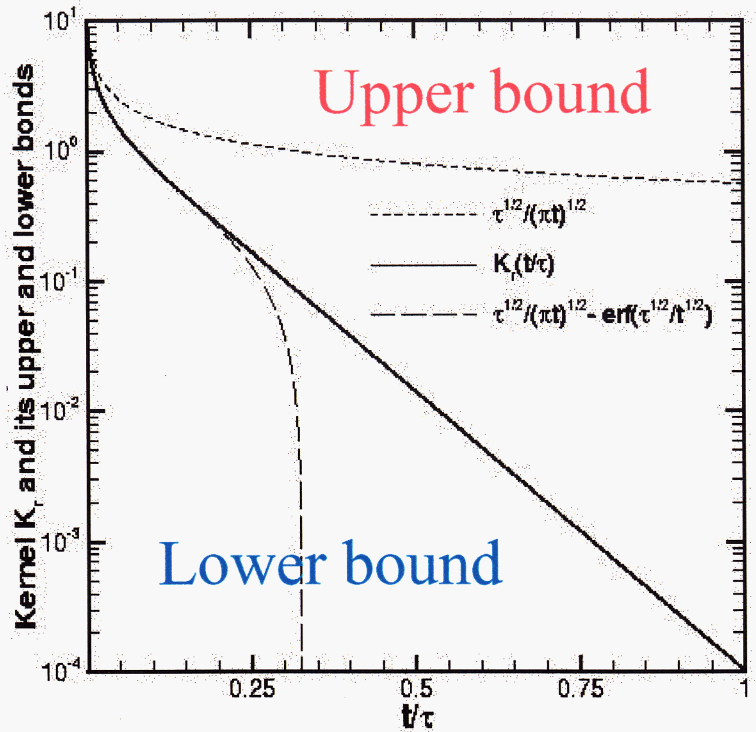


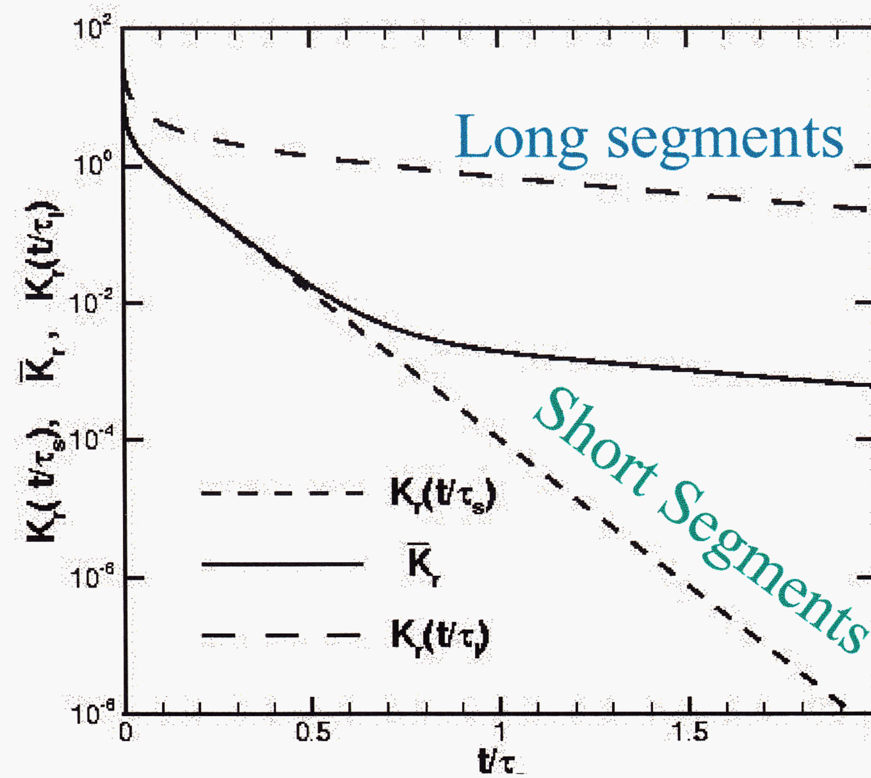
$$\frac{\partial \lambda}{\partial t} = \frac{L^2}{4\tau}\frac{\partial^2 \lambda}{\partial x^2}$$

Where λ is displacement, L is chain length and τ is chain relaxation time.
Chain relaxation time is directly related to chain length, chain elasticity, and friction between other chains.

- Recovers Harlow and Harstad's idea about S.

- Effects of segment length.

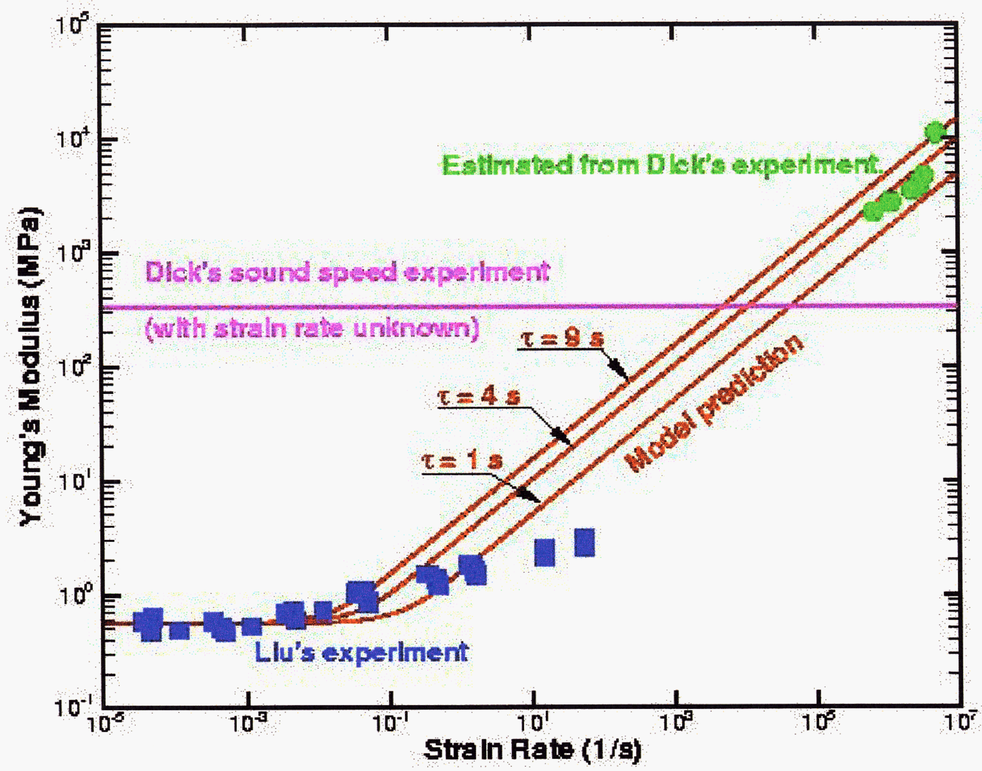




$$\overline{K}_r(t) = \sqrt{\tau_0/t} + \sum_{i=1}^{N} \alpha_i e^{-t/\tau_i}$$

Comparison With Experiment

- No direct data available at high strain rate, so we only be able to compare to indirect data.



Micro-mechanical Approach to Damage and Stiffening

Heuristic approach

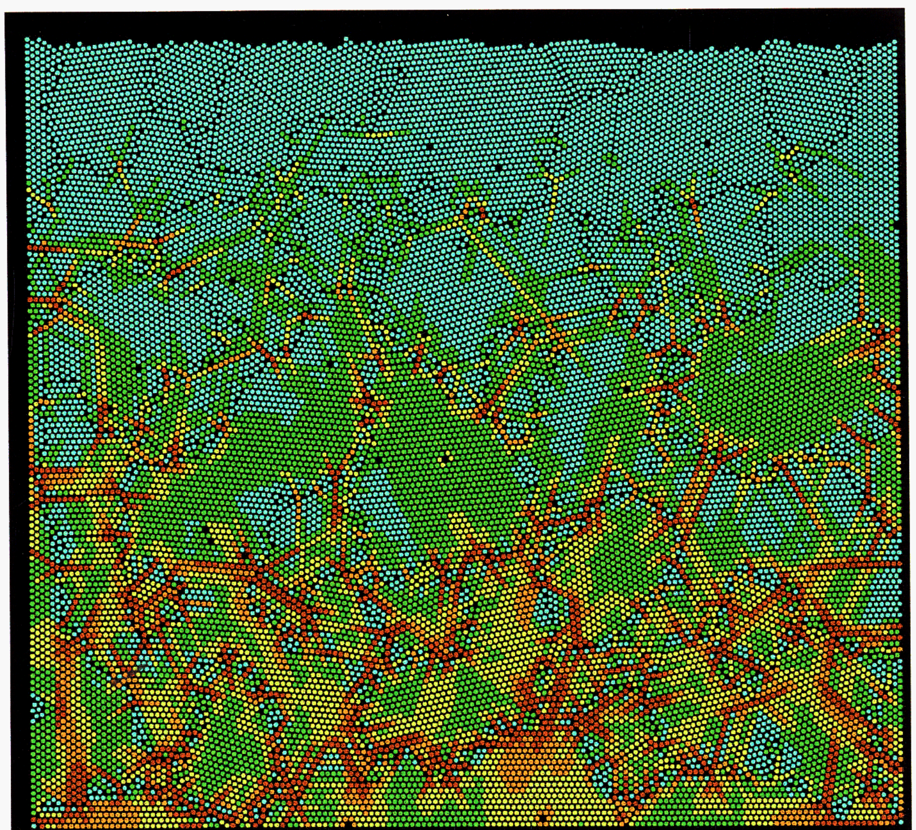
$$E_b = [1 - \alpha(\dot{\varepsilon}) \,|\, \varepsilon \,|^n \,] E_0(\dot{\varepsilon})$$

Confirm or improve the heuristic model for damage.

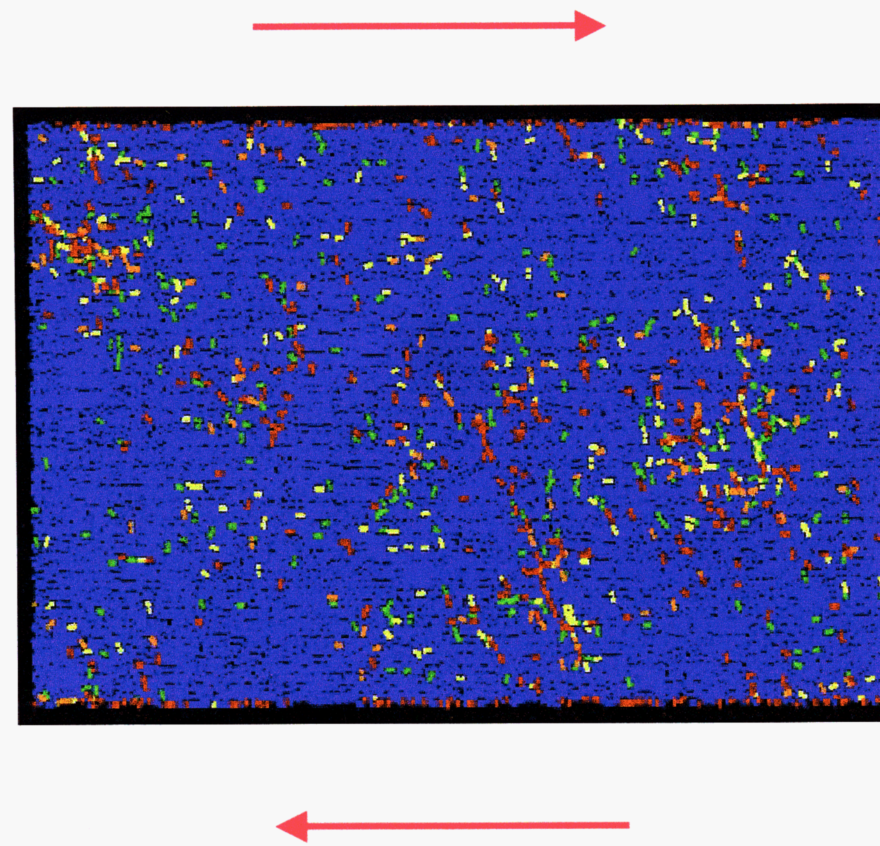
- debonding
- polymer failure
- micro-fracture in crystals
- macro-cracks through the material
- stress bridging

Stress Bridges

Under gravity

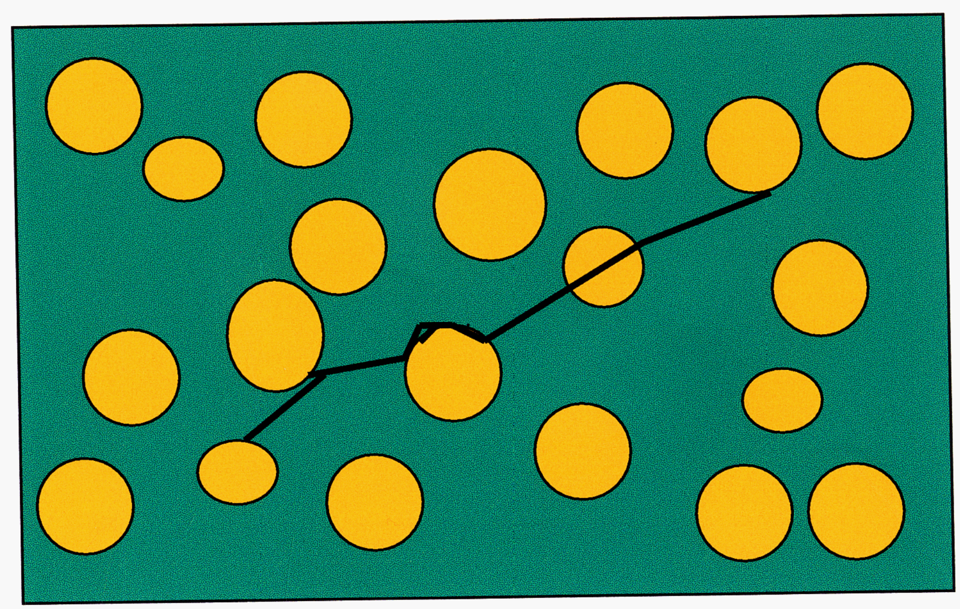


Under shear



Macro-cracks

Direction of Macro-crack Growth is related to cohesive force, local damage of crystal and binder, stain rate, etc.



Current Model for Thermal Effects (With Todd William)

- Spherical entities with distribution of sizes, temperature, velocities, material, stress, …
- PDF describes the distributions.
- Liouville equation for PDF evolution.
- $\dot{T}$ describes local grain heating and local cooling as a results of.
  - Fracture-slip dissipation.
  - Pore collapse.
  - Chemical reactions.
  - Heat conduction from binder to grains.
  - Heat conduction away from hot-spots.

Moments of the PDF

- Macro-stress as a function of macro-strain (agrees with out previous description).
- Thermal-stress effects on constitutive behavior.
- Macro heat energy evolution equation.
- Possible amout of material with $T > T_{initiation}$.
- Probable size of hot spots.
- Probability for ignition.

Summary

- Used statistical micro-mechanical tools to account for crystal-binder interactions.
- Compared our model prediction with experimental results.
- Developed a phenomenological binder stiffening model and a damage model.
- Identified the need for a better binder model.
- Studied polymer models for high strain rate.
- Currently working on micro-physic-based models of damage, thermal processes and macro-crack formation.